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UTILITY PATENT APPLICATION TRANSMITTAL

(Only for new nonprovisional applications under 37 C.F.R. § 1.53(b))

Attorney Docket No.	LAM-P0629
First Inventor or Application Identifier	David Cooperberg, et al.
Title	Method and Apparatus to Calibrate..
Express Mail Label No.	EL575423001US

APPLICATION ELEMENTS
See MPEP chapter 600 concerning utility patent application contents.

ADDRESS TO: Assistant Commissioner for Patents
Box Patent Application
Washington, DC 20231

1. [ ] * **Fee Transmittal Form** *(e.g., PTO/SB/17)*
   (Submit an original and a duplicate for fee processing)

2. [X] **Specification** *[Total Pages* 33 *]*
   (preferred arrangement set forth below)
   - Descriptive title of the Invention
   - Cross References to Related Applications
   - Statement Regarding Fed sponsored R & D
   - Reference to Microfiche Appendix
   - Background of the Invention
   - Brief Summary of the Invention
   - Brief Description of the Drawings *(if filed)*
   - Detailed Description
   - Claim(s)
   - Abstract of the Disclosure

3. [X] **Drawing(s) (35 U.S.C. 113)** *[Total Sheets* 5 *]*

4. **Oath or Declaration** *[Total Pages* [ ] *]*
   a. [ ] Newly executed (original or copy)
   b. [ ] Copy from a prior application (37 C.F.R. § 1.63(d))
      (for continuation/divisional with Box 17 completed)
      [Note Box 5 below]
      i. [ ] **DELETION OF INVENTOR(S)**
         Signed statement attached deleting inventor(s) named in the prior application, see 37 C.F.R. §§ 1.63(d)(2) and 1.33(b).

5. [ ] **Incorporation By Reference** *(useable if Box 4b is checked)*
   The entire disclosure of the prior application, from which a copy of the oath or declaration is supplied under Box 4b, is considered to be part of the disclosure of the accompanying application and is hereby incorporated by reference therein.

6. [ ] **Microfiche Computer Program** *(Appendix)*

7. **Nucleotide and/or Amino Acid Sequence Submission** *(if applicable, all necessary)*
   a. [ ] Computer Readable Copy
   b. [ ] Paper Copy (identical to computer copy)
   c. [ ] Statement verifying identity of above copies

ACCOMPANYING APPLICATION PARTS

8. [ ] Assignment Papers (cover sheet & document(s))
9. [ ] 37 C.F.R.§3.73(b) Statement *(when there is an assignee)* [ ] Power of Attorney
10. [ ] English Translation Document *(if applicable)*
11. [ ] Information Disclosure Statement (IDS)/PTO-1449 [ ] Copies of IDS Citations
12. [ ] Preliminary Amendment
13. [X] Return Receipt Postcard (MPEP 503) *(Should be specifically itemized)*
14. [ ] * Small Entity Statement(s) *(PTO/SB/09-12)* [ ] Statement filed in prior application, Status still proper and desired
15. [ ] Certified Copy of Priority Document(s) *(if foreign priority is claimed)*
16. [X] Other: ..Transmittal Letter.......

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17. If a CONTINUING APPLICATION, check appropriate box, and supply the requisite information below and in a preliminary amendment:

[ ] Continuation [ ] Divisional [X] Continuation-in-part (CIP) of prior application No: _____/_____

Prior application information: Examiner _____ Group / Art Unit _____

18. CORRESPONDENCE ADDRESS

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Signature		**Date**	6/30/2000

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re Application of:) Art Unit:
)
Cooperberg, et al.   ) Examiner:
)
Serial No. [Not yet assigned]   )
)
Filed: June 30, 2000   )
)
For: METHOD AND APPARATUS TO   )
      CALIBRATE A SEMI-EMPIRICAL   )
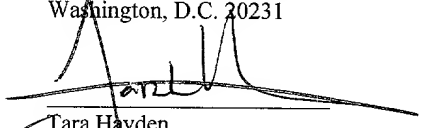   PROCESS SIMULATOR   )

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Tara Hayden

TRANSMITTAL LETTER

Honorable Assistant Commissioner
    for Patents
Box Patent Application
Washington, D.C. 20231

Dear Sir:

Enclosed for filing please find the patent application for an invention entitled,

"METHOD AND APPARATUS TO CALIBRATE A SEMI-EMPIRICAL PROCESS

SIMULATOR", filed on behalf of LAM Research Corporation, assignee from inventors

David Cooperberg, Richard A. Gottscho, and Vahid Vahedi, including Utility Patent

Application Transmittal, 25 pages of specification, 7 pages of claims, 5 sheets of drawing figures, and one page of Abstract.

The attorney's Docket Number is LAM-P0629.

Kindly address all communications regarding this application to:

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No fee is being paid at this time.

Respectfully submitted,
D'ALESSANDRO & RITCHIE

Dated: June 30, 2000

David B. Ritchie
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This application is submitted in the names of inventors David Cooperberg, Richard A. Gottscho, and Vahid Vahedi, both assignors to Lam Research Corporation, a Delaware Corporation.

5

TITLE OF INVENTION

METHOD AND APPARATUS TO CALIBRATE A SEMI-EMPIRICAL

PROCESS SIMULATOR

CROSS-REFERENCE TO RELATED APPLICATIONS

10   This is a continuation-in-part of U.S. Patent Application Serial No. 09/033,997,

filed March 3, 1998 in the names of inventors Maria E. Barone, Richard A.

Gottscho, and Vahid Vahedi and commonly assigned herewith. It is also related to

Applications of a semi-empirical physically based profile simulator, Enhanced

process and profile simulator algorithms filed in common date herewith.

15

BACKGROUND OF THE INVENTION

Field of the Invention

This invention relates to plasma processing of semiconductor devices. In

particular, this invention provides a method and apparatus to calibrate a semi-

20   empirical process simulator for predicting the surface profile and the etch or

deposition rates that a given plasma process will create.

Background Art

Various forms of processing with ionized gases, such as plasma etching and reactive ion etching, are increasing in importance particularly in the area of semiconductor device manufacturing. Of particular interest are the devices used in the etching process. FIG. 1A illustrates a conventional inductively coupled plasma etching system 100 that may be used in the processing and fabrication of semiconductor devices. Inductively coupled plasma processing system 100 includes a plasma reactor 102 having a plasma chamber 104 therein. A transformer coupled power (TCP) controller 106 and a bias power controller 108 respectively control a TCP power supply 110 and a bias power supply 112 influencing the plasma created within plasma chamber 104.

TCP power controller 106 sets a set point for TCP power supply 110 configured to supply a radio frequency (RF) signal, tuned by a TCP match network 114, to a TCP coil 116 located near plasma chamber 104. A RF transparent window 118 is typically provided to separate TCP coil 116 from plasma chamber 104 while allowing energy to pass from TCP coil 116 to plasma chamber 104.

Bias power controller 108 sets a set point for bias power supply 112 configured to supply a RF signal, tuned by a bias match network 120, to an electrode 122 located within the plasma reactor 104 creating a direct current (DC) bias above electrode 122 which is adapted to receive a substrate 124, such as a semi-conductor wafer, being processed.

A gas supply mechanism 126, such as a pendulum control valve, typically supplies the proper chemistry required for the manufacturing process to the interior of plasma reactor 104. A gas exhaust mechanism 128 removes particles from within plasma chamber 104 and maintains a particular pressure within

5   plasma chamber 104. A pressure controller 130 controls both gas supply mechanism 126 and gas exhaust mechanism 128.

A temperature controller 134 controls the temperature of plasma chamber 104 to a selected temperature setpoint using heaters 136, such as heating cartridges, around plasma chamber 104.

10   In plasma chamber 104, substrate etching is achieved by exposing substrate 104 to ionized gas compounds (plasma) under vacuum. The etching process starts when the gases are conveyed into plasma chamber 104. The RF power delivered by TCP coil 116 and tuned by TCP match network 110 ionizes the gases. The RF power, delivered by electrode 122 and tuned by bias match network 120, induces a

15   DC bias on substrate 124 to control the direction and energy of ion bombardment of substrate 124. During the etching process, the plasma reacts chemically with the surface of substrate 124 to remove material not covered by a photoresistive mask.

Input parameters such as plasma reactor settings are of fundamental importance in plasma processing. The amount of actual TCP power, bias power,

20   gas pressure, gas temperature, and gas flow within plasma chamber 104 greatly affects the process conditions. Significant variance in actual power delivered to plasma chamber 104 may unexpectedly change the anticipated value of other

process variable parameters such as neutral and ionized particle density, temperature, and etch rate.

Traditionally, a suite of values of these input parameters suitable for creating a given set of device features has been determined by trial and error.

5   Development of a single process by this empirical approach is costly and time-consuming, requiring treatment of several patterned wafers and subsequent study of the resulting profiles by scanning electron microscopy. Because of the unpredictable way a small change in one input parameter may affect the profile, any modification of the layout--for example, in device dimension, pattern density

10   on the wafer or change in total open area--from one application to another, has often necessitated redevelopment of the process, with the attendant outlay of resources.

Recent advances in device fabrication technology are rendering this approach even more onerous. Decreasing feature sizes demand tighter tolerances

15   on feature dimensions and morphologies, so that the number of trials required to optimize a given process is increasing. The acceleration of wafer diameter growth and the complete redesign of the process involved with an incremental change in diameter have increased the number of times this empirical process must be repeated. The increasing use of devices tailor-made to a specific application also

20   increases the amount of development and optimization activity required.

An alternative, computational approach would derive input parameters from a complete physical description of a plasma process including a plasma

4

model for describing the coupling between the macroscopic input parameters and the macroscopic fluxes, concentrations and energy distributions of the various species in the plasma; and a profile simulator for determining atomistically from the macroscopic fluxes the resulting etch or deposition rate along the wafer surface

5   and calculating the profile evolution therefrom. Ideally, such a physical description of plasma etching and deposition processes would enable the *ab initio* selection of the macroscopic input parameters appropriate for generating a desired profile on the substrate, eliminating the need for expensive and time-consuming test sequences.

10   Research in this field has done much to elucidate mechanisms at work in plasma processes, and thus has contributed scaling laws that could frame a physical description. However, notwithstanding the availability of computational means sufficiently powerful to perform the necessary calculations based on known scaling laws, the implementation of such an *ab initio* approach has been limited by

15   lack of data. For example, the manner in which the values of some coefficients in these laws depend on the particulars of a given process is unknown as yet. In some investigations, determination of the value of such a scaling coefficient consistent with a plasma process defined by a given set of input parameters has been done by comparing a finished profile, created by applying that process, with

20   a simulated profile including one or more of these coefficients as adjustable parameters. Such hindsight evaluation may promote understanding a given coefficient's role in scaling law, but it has not afforded the ability to predict profile

evolution for any process defined by a set of input parameters differing from the set used in the experimental process used to derive the value of that coefficient.

Thus, there is a need for a method for calibrating a semi-empirical process simulator for predicting the surface profiles and the etch or deposition rates that a

5   given plasma process will create.

SUMMARY OF THE INVENTION

A method and apparatus for calibrating a semi-empirical process simulator used to determine process values in a plasma process for creating a desired surface profile on a process substrate includes providing a test model which captures all mechanisms responsible for profile evolution in terms of a set of unknown surface parameters. A set of test conditions is derived for which the profile evolution is governed by only a limited number of parameters. For each set of test conditions, test values are selected and a test substrate is actually subjected to a test process defined by the test values, thereby creating a test surface profile. The test values are used to generate an approximate profile prediction and are adjusted to minimize the discrepancy between the test surface profile and the approximate profile prediction, thereby providing a final model of the profile evolution in terms of the process values.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1A is a block diagram illustrating a plasma etching system.

5   FIG.1B is a flow chart illustrating a first calibration process in accordance with a

specific embodiment of the present invention.

FIG. 2 is a flow chart illustrating a second calibration process in accordance with a

specific embodiment of the present invention.

10

FIG. 3 is an elevational cross-sectional diagram depicting surface kinetics in a

plasma process according to the Langmuir model.

FIG. 4 is a system block diagram illustrating a representative hardware

15   environment in accordance with a specific embodiment of the present invention.

DETAILED DESCRIPTION OF A SPECIFIC EMBODIMENTS OF THE INVENTION

Those of ordinary skill in the art will realize that the following description

5   of the present invention is illustrative only and not in any way limiting. Other

embodiments of the invention will readily suggest themselves to such skilled

persons having the benefit of this disclosure.

A semi-empirical process simulator is a model that seeks to determine the

10   values of input parameters in a plasma process for creating a desired surface

profile on a substrate, such as a semi-conducting wafer. Previous calibration

schemes used in the process simulator relied on fitting the simulation output to test

data gathered near a process window of interest. While useful, this technique is

likely to produce more empirical and less physically based models. An alternative

15   approach to calibration is to design sets of experiments in which the results are

functions of fewer unknown parameters and for which coefficient values can be

derived from best fit to data with greater confidence. The present invention seeks

to improve such calibration process by using models that more faithfully capture

the actual kinetics governing feature evolution and are likely to yield more

20   accurate profile predictions when using reactor settings which may lie outside a

previously calibrated window of operation.

The form of the surface kinetic model for each class of exposed film and class of plasma chemistry may be derived from experimentally observed trends and scalings. Unknown model coefficients however must be calibrated for each specific film and chemistry. A complete surface kinetics model includes equations

5   governing surface coverage and an equation governing etch or deposition rate. Surface reaction rates for the adsorption, desorption, and surface reactions of active neutral species lead to a determination of surface coverage. The mechanisms determining local etch rate will be functions of the computed surface coverage and the ion and neutral flux distributions incident on a feature surface

10   element. Etch mechanisms include physical sputtering due to energetic particle bombardment, chemical assisted sputtering which additionally depends on the surface concentration of one or more etchant species, and thermal etching dependent only on chemical coverages (and surface temperature). Deposition rate is typically defined by the adsorption rate of depositing neutral species.

15

The general procedure to calibrate a semi-empirical process simulator is illustrated in FIG. 1. Free parameters needed to characterize mechanisms such as thermal etching, ion enhanced etching, physical sputtering, and deposition are determined by performing test processes under conditions where only a limited

20   number of such mechanisms contribute to etch or deposition rates and/or surface profiles. The reduced set of unknown surface parameters can then be determined by best fit to etch rate and/or surface profile data collected under these conditions.

In block 100, a test model which captures all mechanisms responsible for profile evolution in terms of a set of unknown surface parameters is provided. The input parameters include descriptors of the pre-processing state of the substrate

5   ("substrate parameters") and quantities defining the operation of a given plasma reactor during the test process ("reactor parameters"). The substrate parameters may include, for example, gross dimensions of the substrate, the distribution and dimensions of any features on the surface, and the substrate composition. The reactor parameters may include any of: power levels, gas temperature, gas

10   pressure, inlet gas composition, and length of time the substrate is treated by the plasma process.

In block 102, a set of test conditions is derived from a subset of the test model defined in block 100 such that only a limited number of unknown surface

15   parameters contribute to the etch or deposition rates and the surface profiles. Such test conditions is derived by adjusting the value of some of the surface parameters to render their effects negligible on the test processes.

For each set of test conditions defined in block 102, surface model

20   unknown parameter test values are yet to be solved for. In block 104, these unknown parameter test values are isolated by eliminating parameters that do not contribute to etch or deposition rates or feature evolution.

The unknown parameter test values of reactor variables and reactor fixed

parameters as selected in block 106, are used in block 108, in which a plasma

model, containing a mathematical description of the plasma in terms of the reactor

parameters for the reactor of interest and coefficients of known or empirically

5   determined value, operates to approximately determine the macroscopic properties

of the plasma generated by the test process. The plasma model characterizes the

species of interest only as belonging to a general class of actors, for example, as

being either charged particles, and thus attracted to the substrate by any applied

bias, or neutral species such as gas molecule and excited radicals. Physical

10   models--for example, Maxwell's and Boltzmann's equations--underlying the

functional dependence in terms of governing experimental input parameters of

such plasma descriptors as particle fluxes, energy, and angular distributions are

well known in the art. (See, e.g., Lieberman and Lichtenberg, *Principles of*

Plasma Discharges and Materials Processing, JohnWiley, 1994). Much is known

15   in the art about how these descriptors scale with the input parameters, based on

such basic physical models in conjunction with experimental data. However, the

absolute value of these fluxes or distributions is not known *a priori* for a given

process. Any such coefficient in the reactor model whose value is unknown is

treated by the calibration as an adjustable parameter or is determined

20   experimentally.

Those macroscopic properties of the plasma can alternatively be determined by measuring the flux distribution at the wafer in a laboratory under the set of test conditions as selected in block 104.

5   In block 112, a profile simulator, containing a mathematical model of the time evolution of the substrate surface profile in terms of the substrate parameters, the macroscopic plasma properties, and coefficients of unknown value, uses the results of block 108 and the substrate parameters provided in block 110 to approximately predict the etch or deposition rates and surface profiles on the

10   substrate. In general, such mathematical model includes a local transport model for calculating fluxes arriving at each point along the substrate surface, a site balance model for calculating the resulting local etch and deposition rates, and a surface advancement algorithm. In a presently preferred specific embodiment of the present invention, a well-known Monte Carlo type approach is used for the

15   local transport.

The site balance model is preferably based on a Langmuir-type model of the kinetics of particle-surface interactions. The model characterizes species that remove material from the substrate as etchants and those that deposit material onto the substrate surface as inhibitors. With reference to FIG. 3, Γ_e and Γ_d respectively

20   represent fluxes of etchants and inhibitors arriving at the surface of the substrate 300. Both etchants and inhibitors react with the surface when they encounter a vacant site. Etchant and inhibitor species react at the surface with respective open-

field reaction coefficients of S_e and S_d to form etchant site 302 and inhibitor site 304. The overall occupancies of the substrate surface sites resulting from reactions with etchant and inhibitor species are represented respectively by fractions θ_e and θ_d, with the number of vacant sites 306 being equal to $1-\theta_e-\theta_d$.

5   Etch products can form and thermally desorb from the surface. Ions arriving at the surface, at flux Γ, can remove etchants that have reacted with the surface by physical sputtering and ion-enhanced etching; arriving ions can also remove inhibitors from the surface by physical sputtering. Taking into account these assumptions and mechanisms, the site balance, in the steady state, for the two

10   types of occupied sites be expressed respectively as

$$\sigma_e \, d\theta_e/dt = \Gamma_e S_e (1-\theta_d-\theta_e) - \theta_e k_{sl}\Gamma_{ie} - \theta_e k_{el}\Gamma_{ie} k_{th,e}\theta_e \cong 0 \text{ and}$$

$$\sigma_d \, d\theta_e/dt = \Gamma_d S_d (1-\theta_d-\theta_e) - \theta_d k_{sl}\Gamma_{ie} \cong 0,$$

15   Wherein k_{el}, k_{sl}, and k_{th} are coefficients, generally of unknown value, associated with the ion-enhanced, physical sputtering and thermal etching mechanisms, respectively. The parameters Γ_{ie} and Γ_{is} are products of ion-enhanced etching and physical sputtering yields, respectively, with ion flux integrated over incident ion energies greater than respective threshold energies, expressed respectively as E_{th}

20   and E_{th}, and over all angles,

$$\Gamma_{ie} = \iint Y_{ie}(\phi,E)\Gamma_i(\phi,E)d\phi dE = \int dE(E^{\frac{1}{2}} - E_{th,e}^{\frac{1}{2}}) \int d\phi \, Y_e(\phi,E) \int_i(\phi,E) \text{ and}$$

$$\Gamma_{is} = \iint Y_{is}(\phi,E)\Gamma_i(\phi,E)d\phi dE = \int dE(E^{\frac{1}{2}} - E_{th,s}^{\frac{1}{2}}) \int d\phi \, Y_s(\phi,E) \int_i(\phi,E).$$

14

This model assumes that the etch yields are products of angular functions and the square root of ion energy, which dependence has been observed experimentally. However, other scaling laws could be used instead. The yield functions only represent functional dependencies, the absolute magnitudes being

5   lumped into the coefficients k's along with other constants.

Expressions for θ_e and θ_d can be derived from the steady-state site balance equation on each type of surface present on the substrate, for example the substrate top and trench bottoms and sidewalls. At each point on the surface, the etch rate,

10   ER, can be written:

$$ER = k_{s2}\,\Gamma_{ls} + \theta_e\,k_{e2}\,\Gamma_{ie} + k_{th}\,\Gamma_e - k_d\,\Gamma_d\,S_d\,(1-\theta_e).$$

The coefficients k_{e2}, k_{s2}, k_d and k_{th} are yield constants associated with physical sputtering, ion-enhanced etching, thermal etching and ion-induced deposition, respectively. Incorporating the expressions for θ_e, θ_d, Γ_{ls} and Γ_{ie} renders the etch

15   rate in terms of the plasma characteristics and the coefficients k, each of which is in principle an adjustable parameter that can be determined by the calibration.

It is also preferred to employ an analytic scheme for surface advancement so that the fine features can be resolved more accurately. One such scheme known in the art and capable of modeling fine feature aspects, such as sharp corners, is

20   the method of characteristics, also known as the shock-front-tracking algorithm. (See, e.g., S. Hamaguchi, "Modeling of Film Deposition for Microelectronic Applications", *Thin Films*, vol. 22, p. 81, S. Rossnagel, ed. Academic Press, San

Diego, 1996). Another is the level set approach. (See, e.g., J.A. Sethian, Level Set Methods: *Evolving Interfaces in Geometry, Fluid Mechanics, Computer Vision, and Materials Science*, Cambridge University Press 1996). The shock-front-tracking approach models the surface (i.e., the interface layer between

5 vacuum and solid) as a collection of piecewise continuous line segments, for each of which a rate of movement is calculated. The possibility of each segment's advancing or receding along its normal independently of the movement of the other segments allows for multiple potential solutions for the resulting surface. In order to avoid multiple solutions, these analytic schemes model the points between

10 the line segments as shocks (i.e., discontinuities in the slope), and properly track the movement of the shocks.

Thus, the cumulative output of blocks 104 through 112, particularly of the operation of the plasma model in block 108 and the profile simulator in block 112,

15 which together comprise an initial mathematical surface profile model as specified above, generates a quantitative but approximate prediction of the etch or deposition rates and surface profile(s) created by the test process.

In block 114, the test values of the input parameters provided in block 104

20 are used to provide a test surface profile, created experimentally by subjecting a test substrate to a test process, in the reactor of interest, defined by the test values of the input parameters. The etch or deposition rates and surface profile(s) of the

test substrate are then measured. In block 116, the etch or deposition rates and surface profile(s) of the test substrate are quantitatively compared with the quantitative approximate prediction resulting from block 112. The difference between the test surface profile(s) and/or etch/deposition rates and the

5   approximate prediction(s) is evaluated according to some criterion, such as an accuracy of range of 10%, applied in block 116.

In general, on the first pass, in which the approximate prediction(s) is computed using preliminary test values of unknown surface parameters, the residual is not sufficiently small to satisfy the criterion, and the calibration

10   procedure advances to block 118, in which the values of the unknown surface parameters are adjusted so as to minimize the discrepancy. The adjusted values are then resubmitted to the profile simulator of block 112 and the plasma model of block 108, for another iteration that render the approximate profile prediction(s) and of the comparison in block 116. Iteration continues until the discrepancy

15   between the test surface profile(s) and the approximate prediction(s) is adequately minimized.

Thus, both block 116 and block 118 effect a calculation of optimum values of the unknown surface parameters test values appearing in the initial

20   mathematical surface profile model. After the surface parameters suitable for the current set of conditions are determined, a different set of conditions in block 104 is selected from block 102 and its respective surface parameters are determined

17

using the same process of block 104 through block 120 until all surface parameters are determined.

For example, physical sputtering yield, energy scaling, and energy threshold coefficients may be obtained by fitting to etch rate data and final profile SEM (Scanning Electron Micrograph) data collected after wafer processing in a chemically inert plasma such an argon discharge with the ion flux and energy distribution to the separately measured or modeled. Coefficients representing thermal etch rate may be obtained by best fit to etch rate data collected under conditions for which there is no energetic ion bombardment. If sufficient gas phase reactant density can be achieve the surface will saturate and the dependence of etch rate on adsorption probability can be eliminated leaving saturated etch rate as the only unknown parameter. Patterned features including overhang structures may be etched in order to isolate surface reaction probabilities which determine transport throughout the feature. In order to calibrate models for deposited material, deposition and etch rates on blanket or patterned wafers processed under conditions favoring deposition may be collected. Incomplete film stacks may be used to isolate the mechanisms leading to redeposition. For chemically assisted sputtering, also referred to as ion-neutral synergy etching, data may be collected from wafers processed under conditions where the ratio of ion energy flux to etchant neutral flux is varied. For large (small) enough ion energy flux to etchant neutral flux ratios the etch rate is dependent only on the etchant flux (incident ion energy flux). Model fits to this etch rate and profile data combined with ion

and/or neutral flux measurements and/or models can be used to determine

unknown coefficients including neutral sticking coefficient, neutral desorption

and/or recombination rates, average etch product stoichiometry, and yield per

incident ion as a function of energy and angle. For all the sets of experiments

5   above subsets of the complete process chemistry may be used to further isolate

and calibrate specific reactions.

        In one presently alternative specific embodiment, the approximate profile

10   prediction generated by the profile simulator in block 112 comprises a series of

frames, each computed after a sufficiently small time increment, and block 114

only compares frames of the approximate profile prediction that correspond to

cumulative exposure times roughly equal to the time of the snapshots in the test

surface profile. If the test profile includes multiple snapshots at different exposure

15   times and/or at a different test value of one or more input parameters other than

time, block 116 compares each test snapshot with the appropriate frame of the

profile prediction and the system operates to minimize the residual over the entire

pairwise comparison.

20   As will now be evident to those of ordinary skill in the art, many

configurations departing from the procedure shown in FIG. 1 fall within the scope

of the invention. For example, FIG. 2 illustrates another specific embodiment in

which block 206 combines the plasma model with the unknown parameter test

values and the substrate parameters in a single module. The entire initial

mathematical surface profile model may reside in a single module, block 206,

rather than being divided into distinct parts 108 (FIG. 1) and 112 (FIG. 1) to deal

separately with phenomena acting over different length scales. Alternatively,

5   depending on the nature of the initial mathematical surface profile model and

comparison algorithm used, insertion of the test values and preliminary surface

parameters into the initial mathematical surface profile model may be delayed

until the comparison block.

10   Turning to FIG. 4, which illustrates, in block-diagram form, a hardware

system incorporating the invention. As indicated therein, the system includes a

system bus 400, over which all system components communicate, a mass storage

device (such as a hard disk or optical storage unit) 402 as well as a main system

memory 404.

15

The operation of the illustrated system is directed by a central-processing

unit ("CPU") 406. The user interacts with the system using a keyboard 408 and a

position-sensing device (e.g., a mouse) 410. The output of either device can be

used to designate information or select particular areas of a screen display 412 to

20   direct functions to be performed by the system.

The main memory 404 contains a group of modules that control the operation of CPU 406 and its interaction with the other hardware components. An operating system 414 directs the execution of low-level, basic system functions such as memory allocation, file management and operation of mass storage

5   devices 402. At a higher level, an analysis module 416, implemented as a series of stored instructions, directs execution of the primary functions performed by the invention, as discussed below. Instructions defining a user interface 418 allow straightforward interaction over screen display 412. User interface 418 generates words or graphical images on display 412 to prompt action by the user, and

10   accepts user commands from keyboard 408 and/or position-sensing device 410. The main memory 404 also includes one or more database 420, in general containing any of the test or process values of input parameters including input variables, the desired profile, the test surface profile and rough preliminary test values in the plasma model and profile simulator.

15

It must be understood that although the modules of main memory 404 have been described separately, this is for clarity of presentation only; so long as the system performs all necessary functions, it is immaterial how they are distributed within the system and its programming architecture.

20

The test surface profile(s) is produced experimentally, as is well known in the art, by subjecting one or more test substrates to a test process(es) in a plasma

reactor and measuring the resulting surface profile using, for example, scanning electron microscopy. The desired and test surface profiles may be supplied to the hardware system in electronic format or as graphic hardcopy, in which case the image(s) is processed by a digitizer 398 before numerical comparison with the

5   approximate prediction. The digitized profile is sent as bitstreams on the bus 400 to a database 420 of the main memory 404. The test surface profile may be stored in the mass storage device 402 as well as in database 420.

As noted above, execution of the key tasks associated with the present

10   invention is directed by analysis module 416, which governs the operation of CPU 406 and controls its interaction with main memory 404 in performing the blocks necessary to provide a final mathematical surface profile model including calibrated optimum test values in the initial surface profile model; and, by further processing based on the final surface profile model and a desired surface profile,

15   to determine process values of one or more input variables governing a plasma process sequence appropriates for creating the desired profile on a process substrate; or, by inserting process values of the input variables into the final mathematical model, to predictively calculate a process surface profile to be created on a process substrate by a plasma process sequence defined by the

20   process values.

In particular, the hardware system depicted in FIG. 3 may be used to implement the calibration procedure illustrated by FIG. 1 as follows. The input

variable test values selected in block 104, the test values of any fixed input parameter, and the test surface profile created in block 114 and, as needed, the desired surface profile and/or process values of interest are provided to the database 420 so that they are available to the analysis module 416. Alternatively,

5   the module 416 may retrieve any of the test values, rough preliminary values and test surface profile data from the mass storage device 402 or user interface 418 in response to a user command. Or, the rough preliminary values may be determined by the module 416, based on the input variable test values, according to a predetermined algorithm.

10

Turning now to FIG. 1, by executing the plasma modeling and profile simulation of blocks 108 and 112, respectively, the module 416 establishes the initial mathematical surface model predicting the profile created by the test process. In block 116, the module 416 (FIG. 4) accesses the test surface profile

15   and compares it with the initial mathematical surface profile model and evaluates the residual according to some predetermined criterion. If the residual is not sufficiently small, the analysis module 416 uses the results of the comparison to adjust the test values of the plasma model and profile simulator in block 118. The new test values are retained in the database 420 for another iteration of the

20   modeling/simulation and comparison blocks. When the test surface profile and approximate prediction are sufficiently similar, the test values used in that final iteration are stored in the database 420 as the optimum values.

The analysis module uses these optimum values of the input variables for computation of process values, which can be loaded into a plasma reactor for production of a device including the desired profile, or for profile prediction as

5   described above.

It will therefore be seen that the foregoing represents a highly extensible and advantageous approach to plasma processing of semiconductor devices. The terms and expressions employed herein are used as terms of description and not of

10   limitation, and there is no intention, in the use of such terms and expressions, of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. For example, the various modules of the invention can be implemented on a general-purpose computer using appropriate software

15   instructions, or on a network of computers, or a multiprocessor computer or as hardware circuits, or as mixed hardware-software combinations (wherein, for example, plasma modeling and profile simulation are performed by dedicated hardware components).

20   While embodiments and applications of this invention have been shown and described, it would be apparent to those skilled in the art having the benefit of this disclosure that many more modifications than mentioned above are possible

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without departing from the inventive concepts herein. The invention, therefore, is not to be restricted except in the spirit of the appended claims.

CLAIMS

What is claimed is:

1.   A method for calibrating a semi-empirical process simulator, said method

comprising:

5   deriving a set of test conditions for which a profile evolution is governed

only by a limited number of parameters;

selecting a plurality of test values for each said set of test conditions;

subjecting a test substrate to a test process defined by said plurality of test

values, thereby creating a test surface profile;

10   generating an approximate profile prediction from said plurality of test

values;

adjusting said plurality of test values to minimize a discrepancy between

said test surface profile and said approximate profile prediction, thereby solving

for said limited number of parameters; and

15   repeating said selecting, subjecting, generating, and adjusting for another

said set of test conditions until said plurality of parameters is determined, thereby

providing a final model of said profile evolution in terms said plurality of

parameters.

20   2.   The method of claim 1, wherein said profile evolution comprises an etch

rate, a deposition rate, and a surface profile.

3.   The method of claim 1, wherein generating said approximate profile

prediction includes using a plurality of preliminary test values.

4.   The method of claim 3, wherein said adjusting said plurality of test values

5   includes changing at least one preliminary test value.

5.   The method of claim 4, further comprising comparing said test surface

profile and said approximate profile prediction.

10   6.   The method of claim 5, further comprising incorporating at least one

changed preliminary test value.

7.   The method of claim 1, wherein said semi-empirical process simulator is

used to determine a plurality of parameters governing a plasma process for

15   creating a desired surface profile on a process substrate.

8.   The method of claim 7, further comprising generating a plurality of

parameters from said final model and said desired surface profile.

20   9.   The method of claim 1, wherein said semi-empirical process simulator is

used to predict a surface profile to be created on a process substrate by a

plasma process defined by a plurality of parameters.

10. The method of claim 8, further comprising generating a prediction of said surface profile from said final model and said plurality of parameters.

5 11. The method of claim 1, wherein said plurality of parameters comprises: a plurality of unknown substrate parameters and a plurality of unknown reactor parameters.

12. The method of claim 11, wherein said plurality of unknown substrate
10 parameters comprises: a dimension of a substrate, a substrate composition, and a distribution of a feature on a surface substrate.

13. The method of claim 11, wherein said plurality of unknown reactor parameters comprises: a power level, a gas temperature, a gas pressure, a
15 gas flow, and a gas composition.

14. The method of claim 1, wherein said plurality of parameters varies with time.

20 15. A method for configuring an apparatus for calibrating a semi-empirical process simulator, the method comprising the steps of:

deriving a set of test conditions for which a profile evolution is governed only by a limited number of parameters;

selecting a plurality of test values for each said set of test conditions;

subjecting a test substrate to a test process defined by said plurality of test

5   values, thereby creating a test surface profile;

generating an approximate profile prediction from said plurality of test values;

adjusting said plurality of test values to minimize a discrepancy between said test surface profile and said approximate profile prediction, thereby solving

10   for said limited number of parameters; and

repeating said selecting, subjecting, generating, and revising for another said set of test conditions until said plurality of parameters is determined, thereby providing a final model of said profile evolution in terms said plurality of parameters.

15

16.   An apparatus for calibrating a semi-empirical process simulator, the apparatus comprising:

a computer memory for storing a desired surface profile;

a computer memory for storing a test surface profile, created by subjecting

20   a test substrate to a test process defined by a respective plurality of parameters;

means for deriving a set of test conditions for which a profile evolution is governed only by a limited number of parameters;

means for selecting a plurality of test values for each said set of test

conditions;

means for subjecting a test substrate to a test process defined by said

plurality of test values, thereby creating a test surface profile;

5   means for generating an approximate profile prediction from said plurality

of test values;

means for revising said plurality of test values to minimize a discrepancy

between said test surface profile and said approximate profile prediction, thereby

solving for said limited number of parameters; and

10   means for repeating said selecting, subjecting, generating, and revising for

another said set of test conditions until said plurality of parameters is determined,

thereby providing a final model of said profile evolution in terms said plurality of

parameters.

15   17.   The apparatus of claim 16, further comprising a computer memory for

storing a preliminary test value, the means for generating an approximate

profile description from the initial surface profile model and the respective

test value employing the preliminary test value.

20

18. A program storage device readable by a machine, tangibly embodying a

program of instructions readable by the machine to perform a method for

calibrating a semi-empirical process simulator, the method comprising:

deriving a set of test conditions for which a profile evolution is governed

5 only by a limited number of parameters;

selecting a plurality of test values for each said set of test conditions;

subjecting a test substrate to a test process defined by said plurality of test

values, thereby creating a test surface profile;

generating an approximate profile prediction from said plurality of test

10 values;

adjusting said plurality of test values to minimize a discrepancy between

said test surface profile and said approximate profile prediction, thereby solving

for said limited number of parameters; and

repeating said selecting, subjecting, generating, and adjusting for another

15 said set of test conditions until said plurality of parameters is determined, thereby

providing a final model of said profile evolution in terms said plurality of

parameters.

19. A program storage device readable by a machine, tangibly embodying a

20 program of instructions readable by the machine to perform a method for

configuring an apparatus for calibrating a semi-empirical process simulator,

the method comprising:

deriving a set of test conditions for which a profile evolution is governed only by a limited number of parameters;

selecting a plurality of test values for each said set of test conditions;

subjecting a test substrate to a test process defined by said plurality of test

5   values, thereby creating a test surface profile;

generating an approximate profile prediction from said plurality of test values;

adjusting said plurality of test values to minimize a discrepancy between said test surface profile and said approximate profile prediction, thereby solving

10   for said limited number of parameters; and

repeating said selecting, subjecting, generating, and revising for another said set of test conditions until said plurality of parameters is determined, thereby providing a final model of said profile evolution in terms said plurality of parameters.

15

ABSTRACT

A method and apparatus for calibrating a semi-empirical process simulator used to determine process values in a plasma process for creating a desired surface profile on a process substrate includes providing a test model which captures all mechanisms responsible for profile evolution in terms of a set of unknown surface parameters. A set of test conditions is derived for which the profile evolution is governed by only a limited number of parameters. For each set of test conditions, test values are selected and a test substrate is actually subjected to a test process defined by the test values, thereby creating a test surface profile. The test values are used to generate an approximate profile prediction and are adjusted to minimize the discrepancy between the test surface profile and the approximate profile prediction, thereby providing a final model of the profile evolution in terms of the process values.

5

10

15

TCP Coil

| 106 | 110 | 114 | 116 |

TCP POWER CONTROLLER

TCP Power Supply

TCP Match Network

118

126

130

132

PLASMA

Gas Supply

PRESSURE CONTROLLER

102

104

Gas Exhaust

124

128

136

WAFER

HEATER

122

136

TEMPERATURE CONTROLLER

BIAS Match Network

BIAS Power Supply

112

134

120

BIAS POWER CONTROLLER

108

100

FIG. 1A

LAM-P0629

TEST MODEL WHICH CAPTURES ALL MECHANISMS RESPONSIBLE FOR PROFILE EVOLUTION IN TERMS OF SET OF UNKNOWN SURFACE PARAMETERS ～ 100

DERIVE SET OF TEST CONDITIONS FOR WHICH ETCH/DEPO RATES + SURFACE PROFILE IS GOVERNED BY ONLY SUBSET OF MODEL WITH FEW UNKNOWN SURFACE PARAMETERS ～ 102

104

FOR EACH SET OF TEST CONDITIONS, PROVIDE SURFACE MODEL UNKNOWN PARAMETER TEST VALUES

106

REACTOR PARAMETERS

108

PLASMA MODEL – PROVIDE FLUX DISTRIBUTION AT WAFER BY (1)MEASUREMENT OR (2)REACTOR MODEL

SUBSTRATE PARAMETERS ～ 110

112

SURFACE PROFILE & ETCH/DEPO RATES SIMULATOR

PROCESS WAFER(S) & MEASURE SURFACE PROFILE + ETCH/DEPO RATE

114

COMPARE – RESIDUAL MINIMIZED?

116

NO → REVISE UNKNOWN SURFACE PARAMETERS

118

YES

ALL SURFACE PARAMETERS DETERMINED?

120

NO

YES

DONE

FIG. 1 B

LAM-P0629

TEST MODEL WHICH CAPTURES ALL MECHANISMS RESPONSIBLE FOR PROFILE EVOLUTION IN TERMS OF SET OF UNKNOWN SURFACE PARAMETERS   ~ 200

DERIVE SET OF TEST CONDITIONS FOR WHICH ETCH/DEPO RATES + SURFACE PROFILE IS GOVERNED BY ONLY SUBSET OF MODEL WITH FEW UNKNOWN SURFACE PARAMETERS   ~ 202

204

FOR EACH SET OF TEST CONDITIONS

206

1. PROVIDE SURFACE MODEL UNKNOWN PARAMETER TEST VALUES
2. PROVIDE SUBSTRATE PARAMETERS
3. PROVIDE REACTOR PARAMETERS SUCH AS FLUX DISTRIBUTIONS OF REACTIVE SPECIES AND ENERGETIC PARTICLES ARRIVINE AT WAFER BY MEASUREMENT OR BY REACTOR MODEL

208

SURFACE PROFILE & ETCH/DEPO RATES SIMULATOR

PROCESS WAFER(S) & MEASURE SURFACE PROFILE + ETCH/DEPO RATE

210

COMPARE – RESIDUAL MINIMZED?   NO   REVISE UNKNOWN SURFACE PARAMETERS

212   214

YES

ALL SURFACE PARAMETERS DETERMINED?   216

NO

YES

DONE

FIG. 2

FIG. 3

406 — CPU

402 — MASS STORAGE DEVICES

DIGITIZER — 422

SYSTEM BUS

DATABASE — 420

ANALYSIS — 416

OPERATING SYSTEM — 414

USER INTERFACE — 418

404

400

SCREEN DISPLAY — 412

POSITION-SENSING DEVICE — 410

KEYBOARD — 408

FIG. 4